

Exact Dirac equation calculation of ionization induced by ultrarelativistic heavy ions

A. J. Baltz

Physics Department, Brookhaven National Laboratory, Upton, New York 11973

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Abstract

The time-dependent Dirac equation can be solved exactly for ionization induced by ultrarelativistic heavy ion collisions. Ionization calculations are carried out in such a framework for a number of representative ion-ion pairs. For each ion-ion pair, the computed cross section consists of two terms, a constant energy independent term and a term whose coefficient is $\ln \gamma$. Scaled values of both terms are found to decrease with increasing Z of the nucleus that is ionized.

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I. INTRODUCTION

In a recent work [1] an exact semiclassical Dirac equation calculation of ionization probabilities was presented. The case considered was colliding Pb + Pb at ultrarelativistic energies. A single electron was taken to be bound to one nucleus with the other nucleus completely stripped. The probability that the electron would be ionized in the collision was calculated as a function of impact parameter, but no cross sections were presented. In this paper the approach of Ref. [1] is extended in order to calculate ionization cross sections for a number of representative cases of collisions involving Pb, Zr, Ca, Ne and H ions. In Section II the exact semiclassical method is reviewed and calculations of impact parameter

dependent ionization probabilities are presented. In Section III the results of the probability calculations are used to construct cross sections for various ion-ion collision combinations in the form

$$\sigma = A \ln \gamma + B \quad (1)$$

where A and B are constants for a given ion-ion pair and γ ($= 1/\sqrt{1-v^2}$) is the relativistic factor one of the ions seen from the rest frame of the other. Comparisons are made with previous ionization calculations. In Section IV the example of Pb + Pb at the AGS, CERN SPS, and RHIC is worked out and the CERN SPS case is compared with data.

II. IMPACT PARAMETER DEPENDENT PROBABILITIES

If one works in the appropriate gauge [2], then the Coulomb potential produced by an ultrarelativistic particle (such as a heavy ion) in uniform motion can be expressed in the following form [3]

$$V(\boldsymbol{\rho}, z, t) = -\delta(z-t)\alpha Z_P(1-\alpha_z) \ln \frac{(\mathbf{b}-\boldsymbol{\rho})^2}{b^2}. \quad (2)$$

\mathbf{b} is the impact parameter, perpendicular to the z -axis along which the ion travels, $\boldsymbol{\rho}$, z , and t are the coordinates of the potential relative to a fixed target (or ion), α_z is the Dirac matrix, α is the fine structure constant, with Z_P and v the charge and velocity of the moving ion. This is the physically relevant ultrarelativistic potential since it was obtained by ignoring terms in $(\mathbf{b}-\boldsymbol{\rho})/\gamma^2$ [3] [2]. As will be shown in Section II, when \mathbf{b} becomes large enough that the expression Eq.(2) is inaccurate, we match onto a Weizsacker-Williams expression which is valid for large b . Note that the b^2 in the denominator of the logarithm in Eq.(2) is removable by a gauge transformation, and we retain the option of keeping or removing it as convenient.

It was shown in Ref. [1] that the δ function allows the Dirac equation to be solved exactly at the point of interaction, $z = t$. Exact amplitudes then take the form

$$a_f^j(t = \infty) = \delta_{fj} + \int_{-\infty}^{\infty} dt e^{i(E_f - E_j)t} \langle \phi_f | \delta(z - t) (1 - \alpha_z) \times (e^{-i\alpha Z_P \ln(\mathbf{b} - \boldsymbol{\rho})^2} - 1) | \phi_j \rangle \quad (3)$$

where j is the initial state and f the final state. This amplitude is in the same form as the perturbation theory amplitude, but with an effective potential to represent all the higher order effects exactly,

$$V(\boldsymbol{\rho}, z, t) = -i\delta(z - t)(1 - \alpha_z)(e^{-i\alpha Z_P \ln(\mathbf{b} - \boldsymbol{\rho})^2} - 1), \quad (4)$$

in place of the potential of Eq.(2).

Since an exact solution must be unitary, the ionization probability (the sum of probabilities of excitation from the single bound electron to particular continuum states) is equal to the deficit of the final bound state electron population

$$\sum_{ion} P(b) = 1 - \sum_{bound} P(b) \quad (5)$$

The sum of bound state probabilities includes the probability that the electron remains in the ground state plus the sum of probabilities that it ends up in an excited bound state. From Eq.(3) one may obtain in simple form the exact survival probability of an initial state

$$P_j(b) = |\langle \phi_j | (1 - \alpha_z) e^{-i\alpha Z_P \ln(\mathbf{b} - \boldsymbol{\rho})^2} | \phi_j \rangle|^2. \quad (6)$$

In principle the ionization probability can be calculated without reference to final continuum states. In practice ionization will be calculated both as a sum of continuum probabilities as well as the deficit of bound state probabilities.

Table I shows the results of ionization calculations for an ultrarelativistic Pb + Pb collision. One of the Pb ions has an electron initially in the ground state. The other is completely ionized. Final state probabilities for the electron are calculated as a function of impact parameter b . Calculations have been carried out with a logarithmic spacing in values of b , with the range of b chosen to go from constant probability of ionization at the low end to $1/b^2$ behavior at the high end. The last column which is the sum of final bound state

(column 3) and final continuum state (column 4) population exhibits a small deficit from unity, presumably mostly from the truncation of the energy sum over excited continuum states or secondarily from the truncation of the bound state sum in the calculations.

Tables II and III show corresponding calculations for Ca + Ca, and Ne + Ne.

III. CROSS SECTIONS

The actual cross section comes from the impact parameter integral

$$\sigma_{ion} = 2\pi \int P(b) b db. \quad (7)$$

As was exemplified in Tables I-III, for each ion-ion case calculation of probabilities was performed at ten impact parameters, in a scheme of sequential doubling. The points ran from an impact parameter small enough that the probabilities were approximately constant with b , to an impact parameter large enough that the probabilities had started to fall off as $1/b^2$. The part of the integral, Eq.(7), over this region from the first to the tenth impact parameter takes the form of sum of nine integrals on a logarithmic scale

$$\begin{aligned} \sigma_{1-10} &= \sum_{i=1,9} 2\pi \int_{b_i}^{b_{i+1}} P(b) b db \\ &\simeq \sum_{i=1,9} 2\pi \langle P(b)b^2 \rangle \int_{b_i}^{b_{i+1}} \frac{db}{b}. \end{aligned} \quad (8)$$

Approximating $\langle P(b)b^2 \rangle$ over each interval by the average of the end points we have (for $b_{i+1} = 2b_i$)

$$\sigma_{1-10} = \pi \ln 2 \sum_{i=1,9} (P(b_i)b_i^2 + P(b_{i+1})b_{i+1}^2). \quad (9)$$

Since the probability goes to a constant at the lowest impact parameter, b_1 , the contribution to Eq. (7) from zero up to b_1 is given simply by

$$\sigma_{0-1} = \pi P(b_1)b_1^2. \quad (10)$$

We now need the contribution from the last point computed, b_{10} , out to where $P(b)$ cuts off. We match a Weizsacker-Williams type calculation to the exact calculation at this b_{10}

in order to determine the normalization for the calculation of probabilities at larger impact parameters and to make the high end cutoff in b . How the calculation in the delta function gauge and the calculation in the Weizsacker-Williams formulation are equivalent at this matching impact parameter b_{10} is presented in Appendix A.

The Weizsacker-Williams expression for a transition probability at a given impact parameter is of the form

$$P_{WW}(b) = \int_{E_B}^{\infty} P(\omega) \frac{\omega^2}{\gamma^2} K_1^2\left(\frac{\omega b}{\gamma}\right) d\omega, \quad (11)$$

with E_B the ground state electron binding energy (a positive number here).

If $b\omega \ll \gamma$ then

$$K_1^2\left(\frac{\omega b}{\gamma}\right) = \frac{\gamma^2}{\omega^2 b^2}, \quad (12)$$

and

$$P_{WW}(b) = \frac{1}{b^2} \int_{E_B}^{\infty} P(\omega) d\omega. \quad (13)$$

At the matching impact parameter, Eqns. (12) and (13) are accurate up to the point where the energy starts to cut off. Thus $\int_{E_B}^{\infty} P(\omega) d\omega$ may be simply determined

$$\int_{E_B}^{\infty} P(\omega) d\omega = b_{10}^2 P(b_{10}). \quad (14)$$

Next recall that to high degree of accuracy

$$\frac{\omega^2}{\gamma^2} \int_{b_{10}}^{\infty} K_1^2\left(\frac{\omega b}{\gamma}\right) b db = \ln\left(\frac{.681\gamma}{\omega b_{10}}\right). \quad (15)$$

Then from Eqns. (7), (11), (14), and (15) the contribution to the cross section for impact parameters greater than b_{10} is

$$\begin{aligned} \sigma_{10-\infty} &= 2\pi \left(\ln\left(\frac{.681\gamma}{b_{10}}\right) \int_{E_B}^{\infty} P(\omega) d\omega - \int_{E_B}^{\infty} P(\omega) \ln \omega d\omega \right) \\ &= 2\pi b_{10}^2 P(b_{10}) \left(\ln\left(\frac{.681\gamma}{b_{10}}\right) - \langle \ln \omega \rangle \right). \end{aligned} \quad (16)$$

$\langle \ln \omega \rangle$ can be evaluated from the empirical observation that at b_{10} , $P(\omega)$ goes as $1/\omega^n$ with $n \simeq 3.8$. One obtains

$$\langle \ln \omega \rangle = \ln E_B + \frac{1}{(n-1)} \quad (17)$$

One now has the full ionization cross section

$$\sigma = \sigma_{0-1} + \sigma_{1-10} + \sigma_{10-\infty} \quad (18)$$

or in the usual form

$$\sigma = A \ln \gamma + B. \quad (19)$$

with

$$A = 2\pi b_{10}^2 P(b_{10}). \quad (20)$$

and

$$B = \pi P(b_1) b_1^2 + \pi \ln 2 \sum_{i=1,9} (P(b_i) b_i^2 + P(b_{i+1}) b_{i+1}^2) \\ + 2\pi P(b_{10}) b_{10}^2 \left(\ln \left(\frac{.681}{b_{10}} \right) - \ln E_B - \frac{1}{(n-1)} \right). \quad (21)$$

The $A \ln \gamma$ term is entirely from the non-perturbative, large impact parameter region and gives the beam energy dependence arising from the impact parameter cutoff at $b \simeq \gamma/\omega$ (see Eqns. (15) and (16)). Despite the form of Eq.(20) A does not really depend on the matching impact parameter b_{10} since b_{10} is in the region where $P(b) \sim 1/b^2$. The B term is independent of beam energy and contains non-perturbative components from the smaller impact parameters.

Table IV shows the results of calculations of the ionization cross section components A and B for symmetric ion-ion pairs. There is good agreement between the cross sections calculated by subtracting the bound state probabilities from unity (first rows) or calculated by summing continuum electron final states (second rows). The agreement with the Anholt and Becker calculations [4] in the literature is good for the lighter species for both A and B . However with increasing mass of the ions the perturbative energy dependent term A decreases in the present calculations whereas it increases in the Anholt and Becker calculations. The greatest discrepancy is for Pb + Pb, with Anholt and Becker being about 60%

higher. Perhaps this discrepancy is due to the fact that Anholt and Becker use approximate relativistic bound state wave functions and the present calculations utilize exact Dirac wave functions for the bound states. Surprisingly, it is the term B (which has the non-perturbative component) where agreement is relatively good between Anholt and Becker and the present calculations of Table IV.

Table V shows results of the calculation of B (multiplied by Z_2^2/Z_1^2) for a number of representative non-symmetric ion-ion pairs. (Since A is perturbative, scaling as Z_1^2 , its value can be taken from Table IV for the various pairs here.) Note that if one goes to the perturbative limit for a Pb target to be ionized (H + Pb or Ne + Pb) then the scaled B values (17,090, 17,030) are some 30% higher than the necessarily perturbative Anholt and Becker value of 13,000. The good agreement of Anholt and Becker with the present calculations for Pb + Pb B seen in Table IV is thus somewhat fortuitous.

IV. AN EXAMPLE

Table VI presents calculated ionization cross sections for Pb + Pb at the AGS, the CERN SPS, and RHIC. CERN SPS data of Pb with a single electron impinging on a Au target has recently been published by Krause et al. [5]. Their measured cross section of 42,000 barns is significantly smaller than the Anholt and Becker calculation (which includes screening in the target Au) of about 63,600 barns. The result of the present Pb + Pb calculation (55,800 to 58,200 barns) does not include screening and should be compared with the corresponding no-screening calculation of Anholt and Becker (83,700 barns). What was essentially the present Pb + Pb result was privately communicated to Krause et al., and they seem to have then assumed that if screening were to be included, then the present calculation should be scaled by the ratio of the Anholt and Becker screened to unscreened results. They comment in their paper, “With screening included [4] and scaled to a Au target, the Baltz value agrees with the σ_i measured in the ionization experiment (4.2×10^4 b).”

V. ACKNOWLEDGMENTS

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APPENDIX A: RELATIONSHIP OF THE δ FUNCTION POTENTIAL TO THE WEIZSACKER-WILLIAMS FORMULATION

The Weizsacker-Williams cross section for a process induced by a heavy ion projectile of charge Z_p , $\sigma_{ww}(\omega)$ is expressed in terms of the photoelectric cross section $\sigma_{ph}(\omega)$ for the same process.

$$\sigma_{ww}(\omega) = 2\pi \int_{b_0}^{\infty} \frac{\alpha Z_p^2}{\pi^2} \frac{\omega}{\gamma^2} \sigma_{ph}(\omega) K_1^2\left(\frac{b\omega}{\gamma}\right) b db \quad (\text{A1})$$

Now since the photoelectric cross section for a process is given by

$$\sigma_{ph}(\omega) = \frac{4\pi^2\alpha}{\omega} \left| \int d^3r \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{e}} \psi_0 e^{i\omega z} \right|^2, \quad (\text{A2})$$

the Weizsacker-Williams amplitude (apart from an arbitrary constant phase) for the process is

$$a_{ww} = \frac{2\alpha Z_p}{\gamma} K_1\left(\frac{b\omega}{\gamma}\right) \int d^3r \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{b}} \psi_0 e^{i\omega z} \quad (\text{A3})$$

Consider the δ function gauge

$$V(\boldsymbol{\rho}, z, t) = -\delta(z - t) \alpha Z (1 - \alpha_z) \ln \frac{(\mathbf{b} - \boldsymbol{\rho})^2}{b^2}. \quad (\text{A4})$$

Its multipole expansion is

$$\begin{aligned} V(\boldsymbol{\rho}, z, t) = & \alpha Z (1 - \alpha_z) \delta(z - t) \\ & \left\{ -\ln \frac{\rho^2}{b^2} \quad \rho > b \right. \\ & + \sum_{m>0} \frac{2 \cos m\phi}{m} \\ & \times \left[\left(\frac{\rho}{b} \right)^m \quad \rho < b \right. \\ & \left. \left. + \left(\frac{b}{\rho} \right)^m \right] \right\}. \quad \rho > b \end{aligned} \quad (\text{A5})$$

For $b \gg \rho$

$$V(\boldsymbol{\rho}, z, t) = \delta(z - t) \alpha Z (1 - \alpha_z) 2 \frac{\rho}{b} \cos \phi. \quad (\text{A6})$$

One may make a gauge transformation on the wave function

$$\psi = e^{-i\chi(\mathbf{r},t)}\psi' \quad (\text{A7})$$

where

$$\chi(\mathbf{r},t) = -2\theta(t-z)\alpha Z \frac{\rho}{b} \cos \phi. \quad (\text{A8})$$

This leads to added gauge terms in the transformed potential

$$-\frac{\partial\chi(\mathbf{r},t)}{\partial t} - \boldsymbol{\alpha} \cdot \nabla\chi(\mathbf{r},t) = 2\delta(z-t)(1-\alpha_z)\alpha Z \frac{\rho}{b} \cos \phi + 2\theta(t-z)\alpha Z \frac{\boldsymbol{\alpha} \cdot \hat{\mathbf{b}}}{b}. \quad (\text{A9})$$

(This is the same transformation as previously carried out without the restriction $b \gg \rho$ to go to the light cone gauge [6].) Here we obtain the light cone gauge potential for $b \gg \rho$

$$V(\boldsymbol{\rho}, z, t) = 2\theta(t-z)\alpha Z \frac{\boldsymbol{\alpha} \cdot \hat{\mathbf{b}}}{b}, \quad (\text{A10})$$

and we then obtain the perturbative amplitude in the light cone gauge

$$a_{cone} = \frac{-2i\alpha Z_p}{b} \int_z^\infty dt \int d^3r \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{b}} \psi_0 e^{i\omega t}. \quad (\text{A11})$$

Integrate over t

$$a_{cone} = \frac{2\alpha Z_p}{\omega b} \int d^3r \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{b}} \psi_0 e^{i\omega z}. \quad (\text{A12})$$

Now consider a_{ww} . For $\gamma \gg b\omega$

$$K_1\left(\frac{b\omega}{\gamma}\right) = \frac{\gamma}{b\omega}, \quad (\text{A13})$$

and Eq. (A3) becomes

$$a_{ww} = \frac{2\alpha Z_p}{\omega b} \int d^3r \psi_f^* \boldsymbol{\alpha} \cdot \hat{\mathbf{b}} \psi_0 e^{i\omega z}. \quad (\text{A14})$$

Thus if one transforms from the delta function gauge to the light cone gauge the amplitude in that light cone gauge is found to be equal to the Weizsacker-Williams amplitude (within an arbitrary constant phase) as long as $b \gg \rho$ and $\gamma \gg b\omega$.

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TABLES

TABLE I. Ionization and Unitarity: Probabilities for Pb + Pb

b(fm)	e_{gr}^-	$\sum_{bnd} e^-$	$\sum_{cont} e^-$	$\sum e^-$
62.5	.4344	.5337	.4399	.9736
125	.4467	.5474	.4228	.9703
250	.4884	.5920	.3788	.9708
500	.5820	.6828	.2907	.9735
1000	.7303	.8165	.1691	.9856
2000	.8899	.9447	.0526	.9973
4000	.97056	.98986	.00987	.99972
8000	.99270	.99777	.00217	.99994
16,000	.998178	.999547	.000529	.999986
32,000	.999545	.999865	.000131	.999996

TABLE II. Ionization and Unitarity: Probabilities for Ca + Ca

b(fm)	e_{gr}^-	$\sum_{bnd} e^-$	$\sum_{cont} e^-$	$\sum e^-$
250	.95335	.96291	.03548	.99839
500	.95351	.96297	.03516	.99812
1000	.95657	.96562	.03278	.99841
2000	.96355	.97170	.02707	.99878
4000	.97583	.98293	.01635	.99927
8000	.99028	.99520	.00462	.99982
16,000	.99760	.99924	.00074	.99998
32,000	.999419	.999830	.000165	.999996
64,000	.9998559	.9999585	.0000404	.9999989
128,000	.9999640	.9999897	.0000100	.9999997

TABLE III. Ionization and Unitarity: Probabilities for Ne + Ne

b(fm)	e_{gr}^-	$\sum_{bnd} e^-$	$\sum_{cont} e^-$	$\sum e^-$
500	.98814	.99058	.00901	.99959
1000	.98816	.99058	.00895	.99952
2000	.98894	.99125	.00830	.99960
4000	.99070	.99278	.00692	.99970
8000	.99383	.99564	.00418	.99982
16,000	.99753	.99878	.00117	.99996
32,000	.999392	.999809	.000186	.999995
64,000	.9998534	.9999572	.0000416	.9999989
128,000	.9999636	.9999895	.0000102	.9999997
256,000	.99999092	.99999740	.00000254	.99999993

TABLE IV. Calculated Ionization Cross Sections Expressed in the Form $A \ln \gamma + B$ (in barns)

	Pb + Pb	Zr + Zr	Ca + Ca	Ne + Ne	H + H
$1 - \sum_{bnd} e^-$	8680	10,240	10,620	10,730	10,770
$A \quad \sum_{cont} e^-$	8450	9970	10,340	10,440	10,480
Anholt & Becker [4]	13,800	11,600	10,800	10,600	10,540
$1 - \sum_{bnd} e^-$	14,190	28,450	38,010	46,080	71,090
$B \quad \sum_{cont} e^-$	12,920	27,110	36,530	44,430	68,780
Anholt & Becker	13,000	27,800	37,400	45,400	70,000

TABLE V. Calculated values of the scaled quantity $(Z_2^2/Z_1^2)B$ for non-symmetric combinations of colliding particles. The second nucleus (Z_2) is taken to be the one with the single electron to be ionized. Since Anholt and Becker cross sections without screening are completely perturbative, their values of B also can be taken from Table IV, and are repeated here for convenient comparison.

	H + Ne	H + Ca	Ca + H	H + Zr	H + Pb	Pb + H
$1 - \sum_{bnd} e^-$	46,150	38,270	70,820	29,440	17,090	67,550
$\sum_{cont} e^-$	44,490	36,790	68,520	28,070	15,680	65,330
Anholt & Becker [4]	45,400	37,400	70,000	27,800	13,000	70,000
	Pb + Ne	Ne + Pb	Pb + Ca	Ca + Pb	Pb + Zr	Zr + Pb
$1 - \sum_{bnd} e^-$	42,560	17,030	34,720	16,870	26,010	16,250
$\sum_{cont} e^-$	41,000	15,690	33,330	15,530	24,730	14,930
Anholt & Becker	45,400	13,000	37,400	13,000	27,800	13,000

TABLE VI. Example: Calculated Ionization Cross Sections For Pb + Pb (in barns)

	AGS $\gamma = 11.3$	CERN $\gamma = 160$	RHIC $\gamma = 23,000$
$1 - \sum_{bnd} e^-$	35,200	58,200	101,400
$\sum_{cont} e^-$	33,400	55,800	97,800
Anholt & Becker [4]	46,700	83,700	151,600
Anholt & Becker (with screening)		63,600	
Krause et al. Pb + Au data [5]		42,000	